ICARUS - A General One-Dimensional Heat Conduction Code

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CIRCULATION CUPY SUBJECT TO RECALL IN TWO WEEKS

July 20, 1984

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Abstract

A computer code for calculating one-dimensional planar, cylindrical or spherical conduction heat transfer is described. The model can account for material phase change (solidification or melting), multiple material regions, temperature dependent material properties and time or temperature dependent boundary conditions. Finite difference techniques are used to discretize the differential equations. The resulting system of tri-diagonal equations are solved using a standard tri-diagonal reduction method. The equations are formulated so that the solution can be fully implicit, fully explicit or a user specified degree of mix.

Six sample problems that compare numerical predictions to analytical solutions are discussed. Operation of the computer code and all input variables are described. Input file listings and typical edits for the six sample problems are given.

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NOMENCLATURE

| | • |
|----------------|--|
| a | - the distance between the first and second nodes in a region |
| A | area; coefficient for the i+1 term in the tri-diagonal equation |
| В | - coefficient for the i term in the tri-diagonal equation |
| c | - specific heat |
| c _p | - specific heat at constant pressure |
| C _V | - specific heat at constant volume |
| C | - coefficient for the i-l term in the tri-diagonal equation |
| F | - radiation view factor |
| Å. F | - gray body form factor |
| h | - specific enthalpy; convection coefficient |
| ${f h_L}$ | - latent heat |
| k . | - thermal conductivity |
| 4 | - the distance between the last two nodes in a region |
| n | - unit normal at a surface; number of cells in a region |
| Р | - heat flux |
| r | - the ratio of successive nodal point spacing |
| S | denotes surface integration in the integral equations; width of a geometry region; at surface of body |
| t | - time |
| T | - temperature |
| $\mathbf{T_b}$ | - the bulk convection temperature in a gap |
| u | - internal energy |

- u''' internal heat generation per unit volume
- v velocity of control volume boundary
- V volume
- x spatial coordinate
- X phase change boundary position
- coefficient in the flux term for the general mixed boundary condition, type 3
- emissivity
- implicit/explicit solution indicator
- P density
- ت Stefan-Boltzmann constant
- v denotes volume integration in the integral equations

Subscripts

- denotes left side of control volume, interface, gap, or phase change front, or the side of smallest spatial position
- m denotes phase change temperature
- o ambient or free-stream value for convection
- denotes right side of control volume, interface, gap,
 or phase change front, or the side of largest spatial position
- denotes a surface quantity
- ambient or free-stream value for radiation

Superscripts

- n denotes value at timestep n
- n+1 denotes value at timestep n+1

I. INTRODUCTION

In numerous heat transfer problems, the geometry can be approximated quite accurately as being one-dimensional. Under this condition, it is advantages to use a one-dimensional heat transfer code as opposed to multi-dimensional codes such as TACO [1] or TRUMP [2]. The computer code ICARUS was developed to allow easy, straight forward modeling of complex one-dimensional systems. The first version of the code was developed in 1974 [3]. Its original application was to problems in the nuclear explosive testing program at the Lawrence Livermore National Laboratory (LLNL). Since then it has undergone extensive revision and has been applied to problems dealing with laser fusion target fabrication, heat loads on underground tests, magnetic fusion switching tube anodes and nuclear waste isolation canisters.

Among its features are:

- o Multiple material regions
- Temperature dependent material properties (thermal conductivity, specific heat)
- o Solid to liquid (melting) and liquid to solid (solidification) phase transitions where volumetric changes are negligible
- o Time and/or temperature dependent boundary conditions
- o Time and/or temperature dependent internal heat generation
- o Implicit or explicit solution
- o User subroutine linkage that allows the user to incorporate specialized models
- o Material gaps across which radiative and convective heat transfer can take place

Finite difference techniques are employed to solve the governing differential equations. Change of phase requires special treatment. Because phase change involves removal (solidification) or addition (melting) of energy, the phase change process will begin at the edge of a material region. When the phase change front is near the edge of a region, the front is treated as a moving constant temperature interface in a fixed nodal point system. When the front is sufficiently far from the edge of a region, the mesh system

is rezoned and a nodal point is attached to the front. Until the front is again close to the edge of the region, a node moves with the front. This produces changes in the cell width around the front necessitating periodic rezoning of the finite difference mesh.

This report includes a description of the mathematical formulation, numerical solution scheme, users manual and sample problems.

II. GOVERNING EQUATIONS AND MODELS

Energy Transport Equation

Consider the material control volume shown in Figure 1. The finite difference mesh is specified such that control volume boundaries lie midway between nodal points. Since a nodal point typically tracks a phase change front, the control volumes associated with the two adjacent nodes change size. Thus, we must account for material flow across the control volume boundary. The integral representation for the conservation of energy on this control volume, neglecting kinetic and potential energies is

$$\rho = \int_{q}^{q} \int_{V} h dv - \rho \int_{S} h(v \cdot n) ds + \int_{S} (q \cdot n) ds = \int_{V}^{U \cdot 1} dv$$
(1)

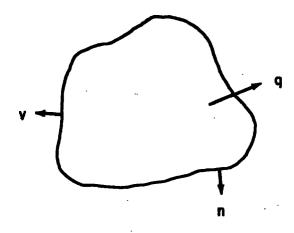


Figure 1. Nomenclature for the general material control volume.

In developing the above equation, we have restricted consideration to solids and liquids where the density can be considered constant, and where

$$c_p \approx c_v = c.$$
 (2a)

Thus

$$dh = cdT. (2b)$$

Using average quantities within the volume integrals, equation 1 becomes

$$\rho \frac{\partial h V}{\partial t} - \rho \int_{B} h(v \cdot n) ds + \int_{B} (q \cdot n) ds = u'' V$$
 (3)

For the one-dimensional systems under consideration, equation 3 becomes

$$PCV \frac{\partial t}{\partial t} + \rho h \frac{\partial V}{\partial t} - [(hvA)_{T} - (hvA)_{L}]$$

$$+ [(qA)_{T} - (qA)_{L}] = u^{111}V$$
(4)

For a control volume whose boundaries are not affected by the phase change front (i.e., v=0) equation 4 reduces to the classic form of the heat conduction equation.

$$\rho_{c}V\frac{\partial T}{\partial t} + [(qA)_{r} - (qA)_{u}] = u'''V.$$
 (5)

The heat fluxes are obtained from Fourier's Law of Conduction where

$$q = -k \forall r . \tag{6}$$

Phase Change Model

A change of phase in a single component material, whether it be solid to liquid (melting) or liquid to solid (solidification) occurs at constant temperature. Thus, there is a constant temperature front that sweeps through the region. The propagation rate of this boundary is given by the so-called Stefan condition [4,5]

where the heat fluxes are again given by Fourier's Law (equation 6).

Equation 7 represents an application of the First Law of Thermodynamics on an infinitesimal control volume containing the phase change zone. The velocities at the control volume boundaries will be

$$v = \frac{1}{2} \frac{dx}{dt}.$$

Gap Model

Material gaps may exist inside a problem where radiative and convective heat transfer are the energy transport mechanisms across the gap. Consider the geometry shown in Figure 2. The energy balances at the left and right edges of the gap are

$$-(Ak \nabla T)_{x} = GA_{x} \stackrel{\wedge}{F}_{x-r} (T_{x}^{4} - T_{r}^{4}) + h_{x}A_{x}(T_{x} - T_{b})$$

$$-(Ak \nabla T)_{r} = GA_{r} \stackrel{\wedge}{F}_{r-x} (T_{x}^{4} - T_{r}^{4}) + h_{x}A_{r}(T_{b} - T_{r})$$
(8)

The terms to the left of the equal signs represent the heat flux on the material side of the edge. The other terms represent the heat fluxes impinging or leaving the surfaces.

The gray body form factor where the geometry is either parallel flat plates, concentric cylinders or concentric spheres and where the spatial dimension increases from left to right (thus $F_{\mu\nu}$ = 1) is given by

$$\frac{A}{F}_{z-r} = \left\{ \frac{1}{\frac{1}{\varepsilon_z} + \frac{A}{A_r} \left[\frac{1}{\varepsilon_r} - 1 \right]} \right\}$$
(9)

The quantities ϵ_{\star} and ϵ_{r} can be specified as functions of temperature.

From reciprocity

$$\hat{\mathbf{F}}_{\mathbf{r}-\mathbf{2}} = \hat{\mathbf{F}}_{\mathbf{2}-\mathbf{r}} \frac{\mathbf{A}_{\mathbf{2}}}{\mathbf{A}_{\mathbf{r}}} \tag{10}$$

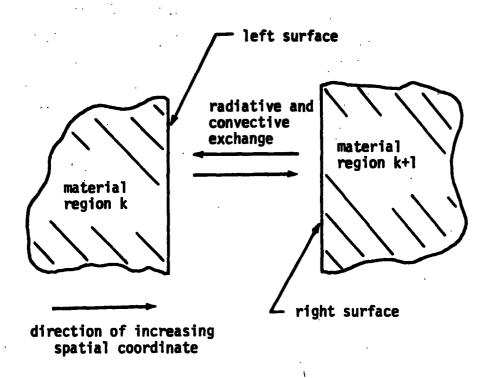


Figure 2. Schematic of a material gap defining orientation, energy exchange processes and terminology.

The bulk convection temperature (T_b) is found by requiring that the heat capacity of the convecting fluid be negligible. Thus,

$$h_{\mu}A_{\mu}(T_{\mu} - T_{b}) = h_{\mu}A_{\mu}(T_{b} - T_{\mu}).$$
 (11)

Boundary Conditions

The boundary conditions available are:

(1) Prescribed temperature. The surface temperature at the boundary is specified to be a constant or a function of time, i.e.,

$$T_{g} = T(t). (12)$$

(2) Prescribed heat flux. The heat flux across the boundary is specified to be a constant or a function of time, i.e.,

$$q_{e} = q(t). \tag{13}$$

A heat flux into the surface is considered positive,

(3) General mixed condition. The heat flux across the boundary is composed of a prescribed heat flux, convection and radiation, i.e.,

$$q_s = \beta q - h_s (T_s - T_o) - \sigma f_{s-\infty} (T_s^4 - T_o^4)$$
(14)

where
$$\hat{F}_{s-\infty} = \frac{1}{(\frac{1}{\epsilon} - 1) + \frac{A_s}{A_m} (\frac{1}{\epsilon} - 1) + \frac{1}{F_{s-\infty}}}$$

The quantities $^{\rm p}$, $^{\rm q}$, $^{\rm T}_{\rm o}$, $^{\rm e}_{\rm s}$, $^{\rm T}_{\rm o}$, $^{\rm h}_{\rm s}$ can be specified as functions of time or the surface temperature. The quantity $^{\rm e}_{\rm r}$ can be specified as a function of time or the reference temperature $^{\rm e}_{\rm o}$.

III. NUMERICAL SOLUTION METHOD

The numerical algorithm incorporates a combined implicit/explicit

formulation to allow the user to specify a fully implicit, explicit or Crank-Nicolson solution type. The resulting system of equations are solved using a tri-diagonal reduction algorithm described by Roache [6].

Equation 5 can be written in the form

where $q^n = -k ^n$ and $q^{n+1} = -k ^n ^{n+1}$

Appropriate values of θ are:

- = 1, fully implicit solution
- = 1/2, Crank-Nicolson solution
- = 0, explicit solution

Using finite difference approximations for the gradients in the heat flux expressions and the time derivative, equation 15 can be cast in the form

$$B_{i}T_{i}^{n+1} = A_{i}T_{i+1}^{n+1} + C_{i}T_{i-1}^{n+1} + D_{i}$$
 (16)

This is the classic tridiagonal form which leads itself to simple, efficient reduction. The subscripts i, i+l and i-l are the difference grid indicies with node i representing the node about which the heat balance is occurring.

IV. SAMPLE PROBLEMS AND VALIDATION

Six sample problems are presented which demonstrate the capability of the code and its accuracy by comparing to analytic solutions. Listings of the input files and sample output are given in Appendix A.

Sample Problem 1 - Two Region Heat Conduction

This problem duplicates a two-material planar thermal system described by

Schneider [7] and Carslaw and Jaeger [4]. The geometry, material properties and boundary conditions are given in Figure 3. The finite difference grid has 25 nodal points, or 24 cell spaces (12 per material region). Results of the calculation are compared to theoretical results in Figure 4. The Fourier number is used to nondimensionalize the results. Even with this relatively coarse grid, the comparison is very good.

Sample Problem 2 - Conduction with Phase Change

This problem duplicates a single material thermal system described by Voller and Cross [8]. The analytic solution is given by Carslaw and Jaeger [4] and Rubenstein [5]. The geometry, material properties and boundary conditions are given in Figure 5. Results of the solution for freezing through four zones are given in Figure 6. The present solution compares well with the numerical solution of Voller and Cross [8] and the analytic solution [4,5].

Sample Problem 3 - Radiatively Cooled Body

This problem duplicates a single material planar system described by Schneider [7]. The geometry, material properties and boundary conditions are given in Figure 7. A comparison of the numerical predictions with the analytical solution is given in Figure 8.

Sample Problem 4 - Linearly Decreasing Heat Flux

This problem duplicates a single material planar system described by Schneider [7]. The geometry, material properties and boundary conditions are given in Figure 9, with a comparison of the calculation to Schneiders curves for temperature increase at the left and right boundaries given in Figure 10.

Sample Problem 5 - Convectively Cooled Sphere

This problem is an example of a solution in spherical geometry. The geometry, material properties and boundary conditions are given in Figure 11. The calculated solution is compared with the analytical solution in Figure 12.

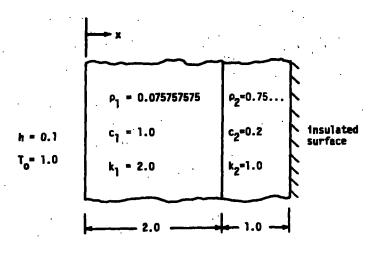


Figure 3. Geometry and material properties for sample problem 1 - two region heat conduction.

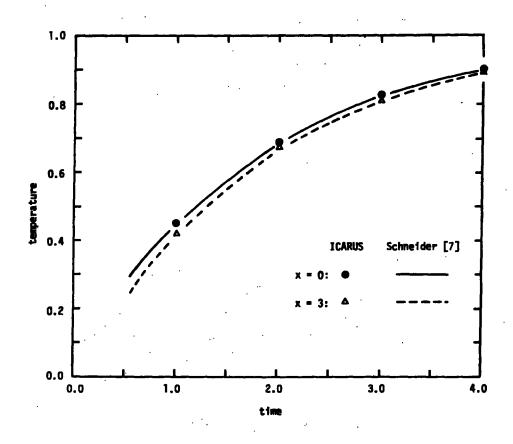


Figure 4. Comparison of sample problem 1 results calculated by ICARUS with the analytical solution taken from Chart 31 of Schneider [7].

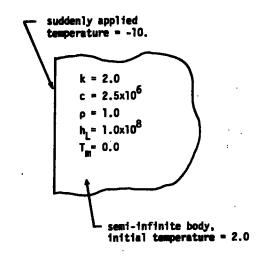


Figure 5. Geometry and material properties for sample problem 2 - conduction with phase change.

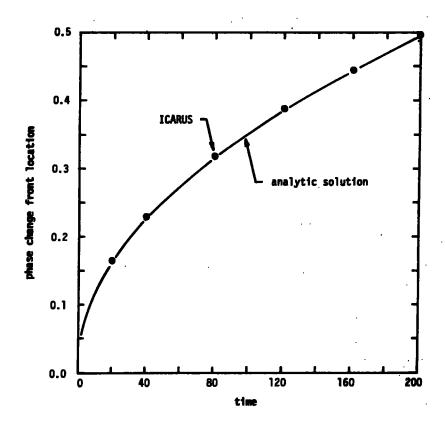


Figure 6. Comparison of sample problem 2 results calculated by ICARUS with the analytical solution presented by Voller and Cross [8].

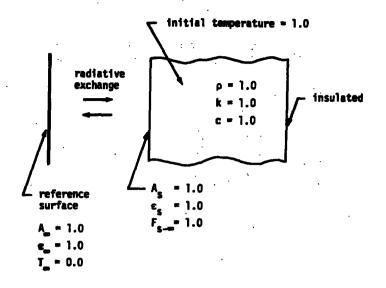


Figure 7. Geometry and material properties for sample problem 3 - radiatively cooled body.

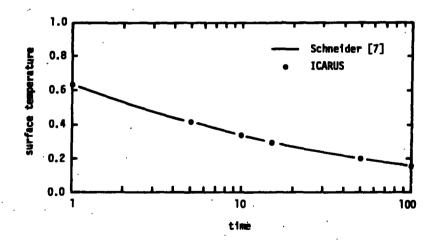


Figure 8. Comparison of sample problem 3 results calculated by ICARUS with the analytical solution taken from Chart 52 of Schneider [7].

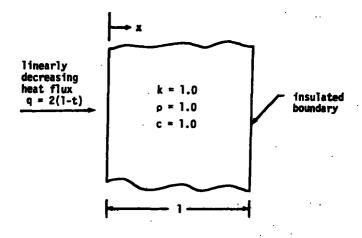


Figure 9. Geometry and material properties for sample problem 4 - linearly decreasing heat flux.

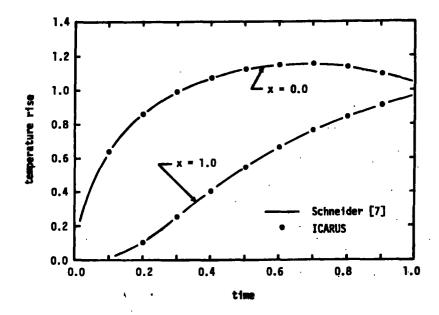


Figure 10. Comparison of sample problem 4 results calculated by ICARUS with the analytical solution taken from Chart 46 of Schneider [7].

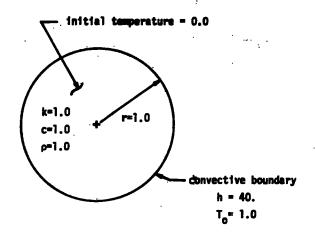


Figure 11. Geometry and material properties for sample problem 5 - convectively cooled sphere.

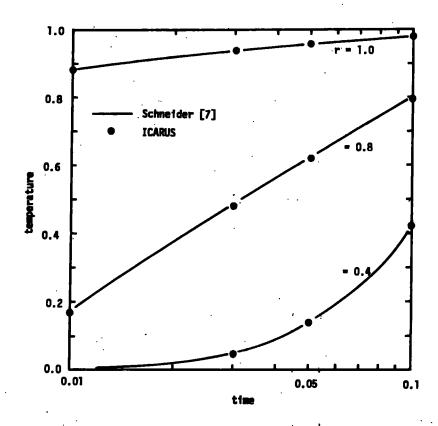


Figure 12. Comparison of sample problem 5 results calculated by ICARUS with the analytical solution taken from Chart 37 of Schneider [7].

できないできることがです。 とればいるとなるとはないないとのできないとからはいてから動きをできないというにはいない

Sample Problem 6 - Infinite Solid Surrounding a Spherical Cavity

The geometry, material properties and boundary conditions for this problem (also in spherical geometry) are described in Figure 13. The calculated solution is compared with the analytical solution in Figure 14.

V. CODE USAGE

Availability

At LLNL, ICARUS is executable on the CDC 7600 computers. The current ICARUS binary file (BICARUS) and executable controllee (ICARUS) are available in the storage take directory

.873512 : NEWICARUS

Execution

The controllee is executed by typing on the computer terminal the line

ICARUS I = inf, R= rtf (1f)

where

inf = input file name

(1f) = denotes the linefeed or return key.

During execution, by typing key words, the user can obtain status information or alter the execution mode of the computer code. The key words and their meanings are:

EDIT (1f) - causes a status message to be printed on the user terminal. An example is given below.

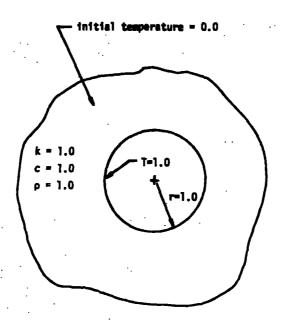


Figure 13. Geometry and material properties for sample problem 6 - infinite solid surrounding a spherical cavity.

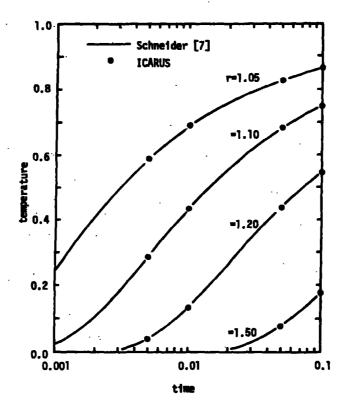


Figure 14. Comparison of sample problem 6 results calculated by ICARUS with the analytical solution taken from Chart 9 of Schneider [7].

END (1f) - causes termination of execution of the computer code. The code will produce a final edit and stop execution in a graceful fashion.

If the problem is a continuation of a previous problem (restart), the code first reads all information contained in the restart file specified on the execute line. Then information contained in input file is read.

The code will produce the following output file families:

HICARUSxxx

the primary edit file containing all edit information and messages. This includes full edits generated at specified intervals and short edits generated at specified intervals. xxx is the family sequence number

Fx105PICAR

- the FR80 plot file. x is the family sequence number.

I CARDUMPOO

- the file that contains restart information. It contains values of all pertinent variables at the time the code is terminated.

Execution Speed

For purposes of estimating computer time usage, the following timing values are given. They include input/output and system times.

without phase change: 1.5×10^{-4} sec node-timestep with phase change: 4.5×10^{-4} sec node-timestep

Program Unit System

Any consistent unit system can be used in ICARUS. The user must, however, exercise caution when solving a radiation problem. The Stefan-Boltzmann constant (SIGMA in namelist 1) must be consistent with the selected unit system. Also, there is no offset temperature feature, so in radiation probems an absolute temperature scale must be used for all references to temperature. This includes temperature input in material and boundary property curves.

VI. INPUT FILE STRUCTURE AND VARIABLE DEFINITIONS

With the exception of the problem title, all information is input via namelists. The input file structure is as follows:

[Namelist O values] SEND [80 character, one line problem title] [Namelist 1 values] SEND [Namelist 2 values] SEND [Namelist 3 values] SEND [Namelist 4 values] SEND [Namelist 5 values] SEND [Namelist 6 values] SEND [Namelist 7 values] SEND

The brackets denote blocks of information that the user places in the file. Sample input listings for the example problems presented in Section IV are given in Appendix A. A brief description of namelist input conventions is given in Appendix B.

For a restart of a previous problem, only those variables whose value the user wishes to change from that given by the restart file need to be specified in the namelists. The input file must contain eight (8) termination cards (SEND).

The input variables are defined below. Values given in brackets denote defaults. Any time a default is not given, a zero value is prescribed. The terms left and right, and upper and lower are used in the descriptions. Left and lower refer to the boundary defined by nodal point number one, which must also be the node having the smallest spatial position. Right and upper refer to the boundary defined by the largest nodal point number, which must also be the node having the largest spatial position. In other words, the spatial position must increase with increasing node number.

Namelist 0 - execution control information

- IREST Denotes execution type
 - = 0, normal initial execution (default)
 - = 1, problem restart

Namelist 1 - General control information

General Operation

- DELTA When the front phase change approaches the edge node of a region, this is the percentage of the cell width from the edge where the edge node is held at the phase change temperature [0.05]
- EPS Convergence limit for nonlinear iteration [10⁻³].
- IGOEM Problem geometry indicator [1]
 - = 1, planar
 - = 2, cylindrical
 - = 3, spherical

IP - Phase change indicator flag

= 0, there is no phase change in this problem (default)

= 1, there is phase change in this problem

ITER - Nonlinear iteration control flag

= 0, do not perform iterations (default)

= 1, perform iterations

ITMAX - Maximum number of iterations to be performed to accommodate nonlinearity [10]

IVEL - Controls application of the boundary motion corrections near a phase change front

= 0, do not include these terms (default)

= 1, include these terms

NCYBUG - Cycle at which the code will stop for user action.

A message is printed to the user terminal when this cycle is reached. This is primarily used as a debugging aid.

SIGMA - The Stefan-Boltzmann constant for radiative heat transfer. Needed only if there is a radiation boundary condition, or radiation gap. [5.66961 x 10^{-8} W/m²K⁴].

THETA - Numerical integration indicator [1.0]

= 0.0, explicit

= 0.5, Crank-Nicolson

= 1.0, Implicit

Geometry

NTEMP - Number of temperature input regions for problem initialization. Maximum of ten. [1]

Time and Timestep Control

DTFAC - Timestep growth factor. The maximum allowable ratio of new timestep to previous timestep $[1 \times 10^{20}]$.

DTFSTART - If other than zero, the timestep to be used to start the phase change motion in a region. Generally not required unless the temperature gradients are very severe.

DTMAX - The maximum allowable timestep

DTMIN - The minimum allowable timestep

DTSTART - Starting timestep for a problem

MAXCYC - Maximum number of cycles. [9999999]

PCHNG - Maximum percentage of a cell width that the phase change front is allowed to transit in one time step.

[0.05]

TMAX - Maximum problem time for this run. Code will terminate if this problem time is reached.

TSTART - Problem start time

Explicit stable timestep criteria are defined in Appendix D.

Edit and Plot Control

General:

- IEDIT1 short edit control flag
 - = 0, produce only cursory edit (default)
 - = 1, produce full diagnotic edit
- IEDIT2 iteration convergence edit
 - = 0, do not produce edit (default)
 - = 1, produce edit
- IFPLOT Phase change front plot flag for plots of location and propagation rate
 - = 0, do not produce plots (default)
 - = 1, produce plots

Hardcopy edit:

- NEDITL Cycle edit frequency for long edits [9999999]
- NEDITS Cycle edit frequency for short edits [9999999]
- TEDITL Time frequency for long edits $[1 \times 10^{20}]$

FR80 plots:

- NPLOT Cycle frequency for FR80 spatial plots [9999999]
- NPOINT Number of nodal points for time history tracking of temperature. Maximum of 10.
- NPTS(j) Nodal point numbers for time history tracking of temperature. Maximum of ten. Required only if NPOINT is non-zero.

NSTORE - Cycle frequency for storing values for FR80 time
history plots. The code can store up to 1000 data points
at each specified node (see NPTS) before producing a
plot.[9999999]

TPLOT - Time frequency for spatial plots [1 x 10²⁰]

Namelist 2 - Problem geometry - specification of material regions

This namelist is used to specify the spatial limits of the problem, the zoning, and the material to be assigned to regions of the problem. A problem may be broken into a maximum of 10 material regions. Spatial limits, nodal point number limits, material number, and geometric zoning factor must be specified for each region. The spatial limits and nodal limits must be sequential (i.e., the node numbers and coordinates for nodes in region j+1 must be greater than for region j, except at the material interface). The total number of nodal points in the problem is given by the value of variable IH for the last region. The first node in the problem must be number one.

NUMREG values must be given for each input variable.

- IH(j) Nodal point value for the right edge at region j. A gap is
 specified between region j and region j+l by making IH(j) =
 IS(j+1) 1. IH(NUMREG) must be no greater than 400.
- IS(j) Nodal point value for the left edge of region j. A gap is
 specified between region j and region j-l by making IS(j) =
 IH(j-1) + 1.
- MATNUM(j) Material number for region number j.
 for j = 1 to 10, input material properties via variables in
 namelist 3
 for j = 11 to 20, specified in the user supplied subroutine
 - RH(j) Coordinate for the right edge of region j.

- RKY(j) Geometric zoning factor for the cells in region j. The ratio between successive zone thicknesses. See appendix C for details.
 - > 1, spacing increases with increasing node number
 - = 1, constant spacing
 - < 1, spacing decreases with increasing node number
- RS(j) Coordinate position for the left edge of region j.

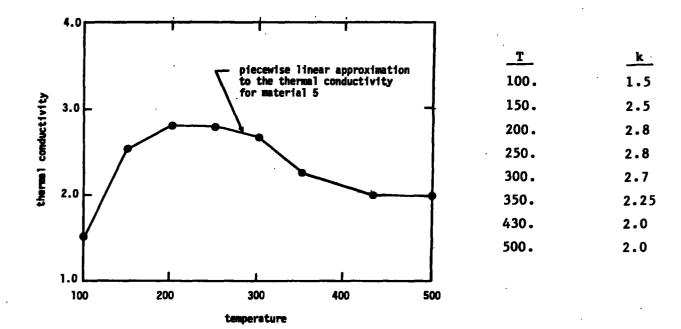
Namelist 3 - Material properties

This namelist is used to specify properties for material numbers one thru ten. Thermal conductivity, specific heat, enthalpy and internal heat generation values are input as a table of entries in a piecewise linear curve. An example is given in Figure 15. Within the computer code, simple linear interpolation is used between entries to find the property value that corresponds to a particular temperature. For temperatures less than the first table entry, the first entry is used. For temperatures greater than the last table entry, the last entry is used.

Thermal Conductivity

- EKM(j,k) Array of thermal conductivity values for material k.

 Values must correspond to increasing temperature. A
 minimum of one value must be given.
- NK(k) Number of values in the thermal conductivity table for material k. At least one.
- TK(j,k) Array of temperature values corresponding to the EKM array for material k. Values must increase with index j. A minimum of one value must be given.



Input deck line specification:

$$NK(5) = 8$$
 $TK(1,5) = 100., 150., 200., 250., 300., 350.$
 $TK(7,5) = 430., 500.$
 $EKM(1,5) = 1.5, 2.5, 2.8, 2.8, 2.7, 2.25$
 $EKM(7,5) = 2.0, 2.0$

Figure 15. Example of Material Property Curve Input

Specific Heat

- CPM(j,k) Array of specific heat values for material k. Values
 must correspond to increasing temperature. A minimum
 of one value must be given.
- NC(k) Number of values in the specific heat table for material k. At least one.
- TC(j,k) Array of temperature values corresponding to the CPM array for material k. Values must increase with index. A minimum of one value must be given.

Enthalpy - input only in phase change problems

- ENM(j,K) Array of enthalpy values for material k. Values must correspond to increasing temperature.
- NE(K) Number of values in the enthalpy table for material k.
- TE(j,K) Array of temperature values corresponding to the ENM array for material k. Values must increase with index.

Internal Heat Generation

Versus temperature:

- NQ(k) Number of values in the internal heat generation rate versus temperature table for material k.
- QGEN(j,k) Array of values of internal heat generation rate versus temperature for material k. Values must correspond to increasing temperature.

TGEN(j,k) - Array of temperature values corresponding to the QGEN array for material k. Values must increase with index j.

Versus time:

- NQT(k) Number of values in the internal heat generation rate versus time table for material k.
- QGT(j,k) Array of values of internal heat generation rate

 versus time for material k. Values must correspond to

 increasing time.
- TIMG(j,k) Array of time values corresponding to QGT for material k. Values must increase with index.

Miscellaneous

- HF(k) Latent heat of material k.
- RO(k) Density of material k.
- TMELT(k) Phase change temperature of material k.

Namelist 4 - Initial temperature distribuition

- AEXP(j) Temperature grading factor for temperature region j.

 Applied in the equation $T = Ax^{AEXP} + B$.
- ITH(j) Upper node value for temperature region j.
- ITL(j) Lower node value for temperature region j.
- TH(j) Temperature at the upper index of temperature region j.

TL(j) - Temperature at the lower index of temperature region j.

Namelist 5 - Boundary conditions

Left Boundary

AR1 - Reference area for radiation heat transfer $(A_{\infty}$ in equation 14). [1.0]

CMULTI(j) - Curve multiplier for property number j. The value extracted from the table for this property is multiplied by this value. See Table I for property definitions.

FORM1 - Radiation view factor for the left boundary. $(F_{s-\infty} \text{ in equation 14})$

LB1 - Boundary condition type for the left boundary [2] = 1, prescribed temperature

= 2, prescribed heat flux

= 3, general mixed boundary condition

NCURV1(j) - Piecewise linear curve number for property number j at the left boundary. See Table I for property definitions.

> 0, time dependent or constant

< 0, temperature dependent

To specify a periodic boundary condition, preced the two digit curve number with a one (1). For example, if property number five (5) is periodic and represented by curve number three (3), specify

Table I

Boundary Property Definitions

| Property Number | Type 1 Boundary Condition | Type 2 Boundary Condition | Type 3 Boundary Condition | | |
|--------------------|---------------------------|---|---|--|--|
| 1 | Surface temperature | Applied surface heat flux | Convective heat transfer coefficient (h _g in eq. 14) | | |
| 2 | - | - | Reference convection temperature (To in eq. 14) | | |
| 3 | - | - | ø in eq. 14 | | |
| 4 | - | - | applied surface heat flux (q in eq. 14) | | |
| 5 | - , | - | reference radiation temperature (T in eq. 14) | | |
| 6 | - | - · · · · · · · · · · · · · · · · · · · | surface emissivity (s _s in eq. 14) | | |
| 7 | - . | - | reference surface emissivity (& in eq. 14) | | |

NCURV1(5) = 103

Right Boundary

- ARM Reference area for radiation heat transfer
 (A_m in equation 14). [1.0]
- CMULTM(j) Curve multiplier for property number j. The value extracted from the table for this property is multiplied by this value. See Table I for property definitions.
- FORMM Radiation view factor for the right boundary. $(F_{a-\infty}$ in equation 14)
- LBM Boundary condition type for the right boundary [2] = 1, prescribed temperature
 - = 2, prescribed heat flux
 - = 3, general mixed boundary condition.
- NCURVM(j) Piecewise linear curve number for property number j at the right boundary. See Table I for property definitions.
 - > 0, time dependent or constant
 - < 0, temperature dependent

To specify a periodic boundary condition, preceed the two digit curve number with a one (1). For example, if property number five (5) is periodic and represented by curve number three (3) we would write

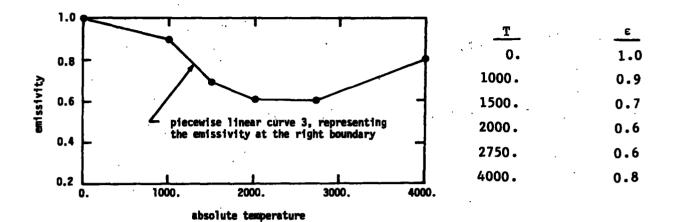
NCURVM(5) = 103

Namelist 6 - Gap parameters

- Note: The numbering convention is such that gap j lies between material regions j and j+1. Where there is no gap specified between regions, the associated parameters are left zero.
- CMEPSL(j) Multiplier for the emissivity curve for the left surface of gap j.
- CMEPSR(j) Multiplier for the emissivity curve for the right
 surface of gap j.
- GHCONL(j) The convection coefficient at the left edge of the gap.
- GHCONR(j) The convection coefficient at the right edge of the gap.
- NCEPSL(j) Curve number describing the emissivity at the left surface of gap j.
 - > 0, time dependent or constant
 - < 0, temperature dependent
- NCEPSR(j) Curve number describing the emissivity at the right surface of gap j.
 - > 0, time dependent or constant
 - < 0, temperature dependent

Namelist 7 - Boundary property piecewise linear curves

Curves describing the boundary properties given in Table I are specified as a table of entries in a piecewise linear approximation to the actual curve. An example is given in Figure 16 for property 6 (surface emissivity) of a type 3 condition at the right boundary. For temperatures or times less than the first table entry, the first entry is used. For temperatures or



In namelist 5:

$$NCURVM(6) = 5$$
 $CMULTM(6) = 1$.

In namelist 7:

$$TCURV(1,5) = 0.$$
 1000. 1500. 2000. 2750. 4000. $VCURV(1.5) = 1.0$ 0.9 0.7 0.6, 0.6 0.8 $NBC(5) = 6$

Figure 16. Example of Boundary Property Piecewise Linear Curve Specification.

times greater than the last table entry, the last entry is used, except in the case of a periodic boundary condition. For a periodic boundary condition, one complete period must be given. VCURV values for the first and last entries must be the same for a periodic boundary property.

- NBC(k) Number of entries in boundary property curve k.
- TCURV(j,K)- The jth time or temperature entry for curve k.

 Corresponds to VCURV(j,k).
- VCURV(j,k)- The jth boundary property entry for curve k.

 Corresponds to TCURV(j,k).

VII. OUTPUT FILE DESCRIPTION

When processed, the information written to the output file has the following structure.

- code title page giving version information and the start time, date and executing computer for the problem
- · input file image
- setup record giving the value of all input variables
- edits at cycle 0 and subsequent cycles as determined by the input edit variables
- · edit at the final cycle
- timing information giving the total execution time and the time accounted for by CPU, system, and I/O operations.

A sample edit is given in Appendix A. The edit is structured as follows:

- problem title
- time information block with

TIME - current problem time

CYCLE - number of timesteps since start of problem

DT - current timestep

NITER - number of non-linear iterations performed during he current cycle

Nodal point state block

I - nodal point number

R - coordinate of nodal point I

DR - nodal point spacing. Distance between nodes I and I + 1

T - Temperature at node I

ITYPE - Equation type for node I

= 1, node interior to a region

= 2, node on a material region interface

= 3, node at the left edge of a gap

= 4, node at the right edge of a gap

MATN - material number

IPHASE - material state indicator

= N, phase change cannot take place at this node

= S, the material phase is currently solid

= L, the material phase is currently liquid

= F, the phase change front is at this node

EK - the thermal conductivity at node I.

CP - the specific heat at node I

QN - the total internal heat generation at node I

ENTH - the enthalpy at node I

Edge and interface state block

REG. NO. - region number

EKL - Thermal conductivity at the left edge of the region

EKR - Thermal conductivity at the right edge of the region

CPL - Specific heat at the left edge of the region

CPR - Specific heat at the right edge of the region

QGL - Internal heat generation at the left edge of the region

QGR - Internal heat generation at the right edge of the region

IPL - Material state indicator for the left edge of the region.

See IPHASE for definition.

IPR - material state indicator for the right edge of the

region. See IPHASE for definition.

ENL - Enthalpy at the left edge of the region

ENR - Enthalpy at the right edge of the region

Phase change front property block (output only if IP = 1)

REG. NO. - Region number

NODCHG - node associated with the front

IFRONT - denotes front model

= 0, node stationary. Used at edges of region

= 1, node moves with front

EKFL - Thermal conductivity to the left of the phase change front.

EKFR - Thermal conductivity to the right of the phase change front.

CPFL - Specific heat to the left of the phase change front.

CPFR - Specific heat to the right of the phase change front.

ENFL - Enthalpy to the left of the phase change front.

ENFR - Enthalpy to the right of the phase change front.

Phase change front propagation block (output only if IP = 1)

REG. NO. - Region number

RFRONT - Position of the phase change front

DFRONT - Position change of the phase change front during the last cycle.

RATE - The rate of change in the position of the phase change front.

PCNT - A parameter characterizing the mesh irregularity at the phase change front. The ratio of the mesh spacing right of the phase change front to the mesh spacing left of the phase change front.

QI - The quantity q in equation 7.

QO - The quantity q in equation 7.

QNET - The quantity (QI - QO)

DMASS - The mass that underwent phase change during the last cycle.

DVOL - The volume that underwent phase change during the last cycle.

Timestep control block

DT - The current timestep.

DTMAX - The maximum allowable timestep.

DTMIN - The minimum allowable timestep.

DTF - The minimum timestep allowed by phase change front propagation considerations.

- DTA The maximum timestep allowed by phase change temperature approach considerations.
- DTE The maximum explicit timestep.

VIII. ACKNOWLEDGMENTS

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IX. REFERENCES

- 1. P. J. Burns, "TACO2D A Finite Element Heat Transfer Code," LLNL, UCID-17980, Rev. 2 (1982).
- 2. A. L. Edwards, "TRUMP: A Computer Program for Transient and Steady-State Temperature Distributions in Multidimensional Systems," LLL, UCRL-14754, Rev. 3 (1972).
- 3. S. B. Sutton, "ICARUS A Multi-option Generalized One-dimensional Heat Transfer Code," LLL, UCIR-1125 (1974).
- 4. H. S. Carslaw and J. C. Jaeger, The Conduction of Heat in Solids. Oxford University Press, Oxford (1959).
- 5. L. Rubenstein, "The Stefan Problem," Transactions in Mathematics Monograph No. 27, American Mathematical Society (1971).
- 6. P. J. Roache, Computational Fluid Dynamics, Hermosa Publishers, Albuquerque (1972).
- 7. P. J. Schneider, Temperature Response Charts, John Wiley, New York (1963).
- 8. V. Voller and M. Cross, "An Explicit Numerical Method to Track a Moving Phase Change Front," Int. J. Heat Mass Transfer, Vol. 26, No. 1, pp. 147-150 (1983).

Appendix A

Sample Problem Input File Listing

Following are input listings and example edits for the sample problems. In the input file listing, lines with a leading asterisk are treated as comment lines by the computer.

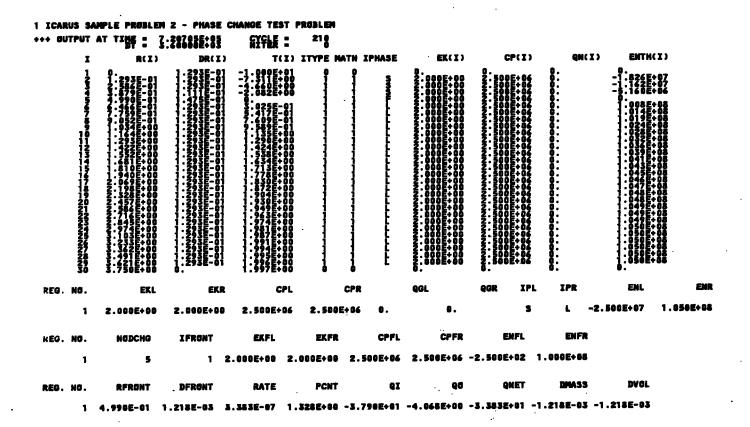
Sample Problem 1 - Two-region Heat Conduction

Input file:

| 1 ICARUS S | MPLE PROBLE | N 1 - THS RE | DIGN HEAT CO | NBUCTION | | | | | | | | |
|---|--------------|--|--------------|-------------|--------|---------------------------------------|------|------|--|-----|---------|-----|
| +++ GUTPUT | AT TIME : | 7.50100E-01 1.00000E-04 | CYCLE : | 7501 . 0 | | | | | | | | |
| I | R(I) | DR(I) | T(I) | ITYPE MATN | IPHASE | EK(I) | • | P(I) | QN | (I) | ENTH(I) | |
| 1,000456-00-00-00-00-00-00-00-00-00-00-00-00-00 | 2.22.22. | 22.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2 | | G | | 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | | | 99999999999999999999999999999999999999 | | | |
| REG. NO. | EKL | EKR | CPL | CPR | | QOL | QGR | IPL | IPR | | ENL | ENR |
| 1 | 1:000E+00 | 1:000E+01 | 1:000E+00 | 1:000E+00 | 8: | 0 . | | N | N | 8: | 8: | |
| | DT | DTMAX | DTMIN | DTF | | DTA | DTE | | | | | |
| | 1.0000E-04 | 1.8000E-04 | 0. | 1.0000E+20 | 1.0000 | E+20 2.1701 | E-05 | | | | | |

Sample Problem 2 - Conduction with Phase Change

Input file:



Sample Problem 3 - Radiatively Cooled Body

Input File:

```
1 ICARUS SAMPLE PROBLEM 3 - RADIATION AT LEFT BOUNDARY (SCHNEIDER CHART $2)

*** OUTPUT AT TIME * 1.00000E-02 CYCLE * 2000

IT R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

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1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

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1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

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1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ENTH(I)

1 R(I) DR(I) T(I) ITYPE MATH IPHASE EX(I) CP(I) QN(I) ITYPE EXTENSION IN INTERPRETATION IN INTERPRETATION IN INTERPRETATION IN INTERPRETATION INTERPRETATION IN INTERPRETATION INTERPRETATION IN INTERPRETATION INTERP
```

Sample Problem 4 - Linearly Decreasing Heat Flux

Input File:

Sample Problem 5 - Convectively Cooled Sphere

Input File:

Sample Problem 6 - Infinite Solid Surrounding a Spherical Cavity

Input File:

Example Edit:

| 1 ICARUS SAMPLE PROBLEM 6 - SOLID AROUND SPHERICAL CAVITY (SCHNEIDER 09) | | | | | | | | | |
|--|--|--|------------|---------|-------------|---------|-------|---|--|
| +++ GUTPUT AT TIME . | 1:80800E-01 | exeft : | 1000 | | | | | | |
| I RCI | | | ITYPE MATN | IPHASE | EK(I) | CP(I) | QN(I) | ENTH(1) | |
| | CHANNAMANNA CARACTERIA CONTROL CARACTERIA CONTROL CARACTERIA CONTROL CARACTERIA CARACTER | 3334444444444478888888888884846666666666 | | | | | | 000000000000000000000000000000000000000 | |
| REG. NO. EKL | | CPL | | | QGL | QGR IPL | | ENL | |
| 1 T.000E+00 | | | | | | N | M 0. | | |
| PT | | DTMIN | | | | DTE | | | |
| 1.0000E-04 | 1.8000E-84 | •. | 1.0000E+28 | 1.00000 | E+20 3.1250 | E-04 | | | |

Appendix B

Namelist Input Conventions

In namelist input, no formats are employed. The actual variable name employed in the computer code is used in the input file. Values are equated to the variable name. For example, if we want the variable TMAX to have the value 5.37, we merely place in the input file the statement

TMAX = 5.37

Dimensional variables must be specified in a slightly more controlled fashion. If we want the fifth, sixth and seventh members of vector variable NBC to be 5, 10 and 3, we would place in the input file the statement

NBC(5) = 5 10 3

where values are space delimited. This input form operates as an implied do-loop where the starting loop value is given, and as many values as are given are placed in successive storage locations.

For a doubly dimensioned vector, storage is performed columnwise as demonstrated in Table B-1. Thus, implied looping is performed easily only on the leading index. As an example, consider the thermal conductivity for material number six (6) where we want the third, fourth, fifth, sixth and seventh entries to be 1.0, 1.1, 1.5, 2.3 and 3.1. We would place in the input file the statement

EKM(3,6) = 1.0 1.1 1.5 2.3 3.1

For this particular variable, the first index denotes the table entry position for the material and the second index the material number.

Table B-1

Columnwise storage sequence for an array declared as A(3,3)

Element Location A(1,1) 1 A(2,1) 2 A(3,1) 3 A(1,2) 4 A(2,2) 5 A(3,2) 6 A(1,3) 7 A(2,3) 8

A(3,3)

Appendix C

Geometric Zoning Relations

To determine the necessary input parameters (grading factor and number of nodes) in a region that is geometrically zoned the following relations [C-1] are applied

$$\frac{x}{a} = r^{n-1} \tag{C-1}$$

$$r = \frac{s - a}{s - k} \tag{C-2}$$

$$n = \frac{\ln(x/a)}{\ln r} + 1 \tag{C-3}$$

$$\frac{a}{s} = \frac{r-1}{r^{n}-1} \tag{C-4}$$

where

a = spacing between the first two nodes of the region

= spacing between the last two nodes of the region.

n = total number of spaces in the region

r = ratio of adjacent node spacings

s = total length of the region.

If r>1, the spacing increases with increasing index. If 0 < r < 1, the spacing decreases with increasing index. If r=1, the spacing is constant.

These equations must be applied in a particular fashion to evolve a consistent set of parameters. Following are three sequences.

Given s, a, 4:

- Calculate r from equation C-2.
- Calculate n from equation C-3. Generally a non-integer number will result in the evaluation of equation C-3. Round the result to the nearest integer. The quantities a and & will be modified somewhat by the code.

Given s, a, r:

- Calculate # from equation C-2.
- Calculate n from equation C-3. Generally, a non-interger number will result in the evaluation of equation C-3. Round the result to the nearest integer. The quantities a and * will be modified somewhat by the code.

Given s, n, a:

• Calculate r iteratively from equation C-4.

References for Appendix C

C-1. Selby, S. M. (editor), <u>Standard Mathematical Tables</u>, The Chemical Rubber Co., Cleveland (1969).

Appendix D

Explicit Stability Conditions

Several methods for evaluating the timestep stability conditions for the explicit solution of a partial differential equation have been proposed [D-1]. In all instances, the diffusion limit on the timestep is found to be

$$\Delta_{\mathsf{L}} < \frac{1}{2} \, \frac{\Delta_{\mathsf{L}}}{a} \tag{D-1}$$

where the timestep

4r = the grid spacing

 α = the thermal diffusivity (k/ ρ_c)

In problems where properties vary through space or the grid spacing is not uniform, equation D-1 represents a local quantity. To assure stability of a problem in an explicit solution, the minimum of these local conditions must be applied. For an explicit solution, ICARUS calculates the local quantities and selects the minimum.

Reference for Appendix D

D-1. P. J. Roache, <u>Computational Fluid Dynamics</u>, Hermosa Publishers, Albuquerque (1972).